Supporting Information

Structure-Property Relationships in Heteroatom-Doped g-C_3N_4 Nanocarriers for Cimetidine: A Computational Study

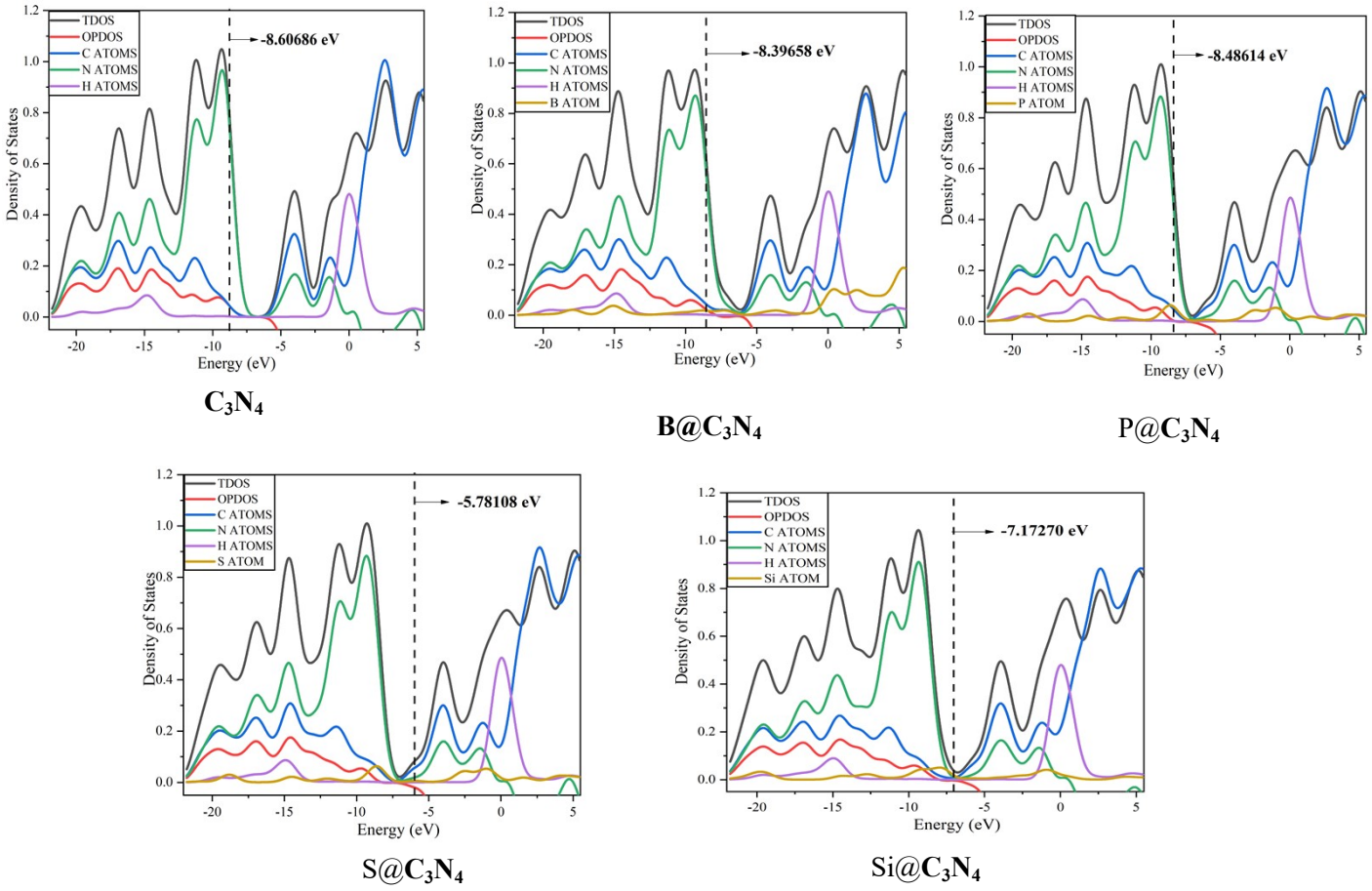

Figure S1. Density of states (DOS) spectra for pristine and X-doped C_3N_4 surfaces, illustrating the effects of heteroatom doping on electronic structure, band alignment, and surface reactivity.

Table S1. NBO second-order perturbation energies ($E^{(2)}$), donor–acceptor interactions and associated orbital transitions for pristine and X-doped C_3N_4, highlighting key charge-transfer pathways.

Compound	Donor	Acceptor	$E^{(2)}$ kcal/mol	E(j)-E(i) a.u	F (i,j) a.u	Transitions

			Surfaces			
B@C_3N_4	N_{53}	C_9-N_{49}	22.42	0.35	0.081	LP→π*
	N_{21}	C_{12}-N_{50}	21.57	0.34	0.077	LP→π*
	N_{53}	C_{10}-N_{46}	20.43	0.36	0.078	LP→π*
C_3N_4	N_{54}	C_9-N_{49}	22.29	0.35	0.081	LP→π*
	N_{53}	C_{16}-N_{41}	21.95	0.35	0.080	LP→π*
	N_{53}	C_{14}-N_{43}	20.68	0.36	0.079	LP→π*
P@C_3N_4	P_{54}	C_{16}-N_{41}	106.82	0.14	0.123	LP→π*
	P_{54}	C_{15}-N_{45}	101.04	0.15	0.122	LP→π*
	P_{54}	C_{14}-N_{43}	100.44	0.15	0.121	LP→π*
S@C_3N_4	C_{17}	C_{14}-N_{40}	101.29	0.08	0.120	LP→π*
	N_{45}	C_{15}-N_{44}	85	0.10	0,118	LP→π*
	C_{17}	C_{16}-N_{41}	31.24	0.13	0.088	LP→π*
Si@C_3N_4	N_{53}	C_9-N_{49}	11.14	0.35	0.081	LP→π*
	N_{53}	C_8-N_{51}	10.52	0.36	0.076	LP→π*
	N_{51}	C_8-N_{53}	9.29	0.60	0.095	LP→ σ*
			Interactions			
Cmt-B@C_3N_4	N_{53}	C_{63}-C_{64}	46.62	0.43	0.129	LP→π*
	C_{55}-C_{59}	C_{56}-N_{73}	26.23	0.25	0.72	π→π*
	O_{75}	C_{74}-N_{76}	24.56	0.62	0.111	LP→ σ*
Cmt-C_3N_4	O_{83}	C_{81}-O_{82}	45.95	0.33	0.111	LP→π*
	O_{82}	C_{81}-O_{83}	29.77	0.61	0.122	LP→π*
	C_{58}-C_{59}	C_{57}-N_{73}	26.83	0.26	0.076	π→π*
Cmt-P@C_3N_4	N_{53}	C_{63} - C_{64}	14.66	0.42	0.072	LP→π*
	C_{64} - H_{70}	C_{10} - N_{53}	1.08	0.79	0.026	σ→σ*
Cmt-S@C_3N_4	C_{17}	C_{14}-N_{40}	108.20	0.08	0.121	LP→π*
	N_{45}	C_{15}-N_{44}	86.56	0.10	0.118	LP→π*
	C_{17}	C_{16}-N_{40}	31.10	0.12	0.087	LP→π*
Cmt-Si@C_3N_4	N_{44}	C_{13}-N_{43}	111.86	0.12	0.149	LP→π*
	C_{14}	Si_{54}	82.29	0.16	0.150	LP→LP*
	C_{13}-N_{43}	C_{14}	50.28	0.14	0.128	π→LP

Table S2. Mulliken atomic charge distribution of isolated cimetidine (Cmt) and adsorbed cimetidine on pristine and X-doped C_3N_4 surfaces (X = B, P, S, and Si). The calculated charges provide insight into charge redistribution and electron transfer occurring during adsorption.

Atoms	**Cmt/e**	**Cmt-C_3N_4/e**	**Cmt-B@C_3N_4/e**	**Cmt-P@C_3N_4/e**	**Cmt-S@C_3N_4/e**	**Cmt-Si@C_3N_4/e**

C1	0.020	0.024	0.031	0.105	0.017	0.026
C2	0.050	0.044	0.043	0.009	0.049	0.049
C3	0.012	0.002	-0.004	-0.108	0.017	0.004
C4	0.178	0.175	0.181	0.116	0.171	0.168
C5	-0.015	-0.006	0.000	-0.042	-0.014	0.002
C6	0.059	0.058	0.058	0.101	0.051	0.063
C7	-0.011	-0.018	-0.036	-0.014	-0.014	-0.027
C8	0.069	0.068	0.078	0.056	0.068	0.077
C9	0.021	0.030	0.030	-0.003	0.038	-0.008
C10	0.016	0.034	0.109	0.005	-0.043	0.081
C11	-0.009	-0.024	-0.044	-0.006	0.027	-0.043
H12	0.019	0.022	0.020	-0.007	0.021	0.018
H13	-0.014	-0.012	-0.003	-0.002	-0.007	0.001
H14	-0.009	-0.010	-0.015	-0.024	-0.013	-0.012
H15	-0.007	-0.004	-0.003	-0.002	-0.014	-0.004
H16	-0.002	-0.010	-0.063	0.006	0.047	0.011
H17	-0.018	-0.010	-0.007	-0.016	-0.027	-0.016
Cl18	-0.093	-0.088	-0.083	-0.085	-0.089	-0.083
N19	-0.162	-0.167	-0.167	-0.115	-0.165	-0.168
C20	0.133	0.137	0.149	0.155	0.137	0.149
O21	-0.172	-0.171	-0.179	-0.339	-0.184	-0.179
N22	-0.234	-0.233	-0.232	-0.121	-0.231	-0.234
H23	0.124	0.125	0.127	0.143	0.127	0.127
C24	0.167	0.165	0.163	0.186	0.165	0.163
H25	0.031	0.033	0.035	0.043	0.034	0.036
H26	0.048	0.049	0.052	0.050	0.045	0.053
C27	0.113	0.114	0.114	0.103	0.115	0.114
O28	-0.227	-0.226	-0.225	-0.219	-0.223	-0.226
O29	-0.199	-0.199	-0.198	-0.185	-0.199	-0.197
H30	0.186	0.187	0.188	0.175	0.188	0.188
O31	-0.262	-0.264	-0.247	-0.176	-0.264	-0.241
H32	0.188	0.187	0.195	0.202	0.176	0.185
Total	0.000	0.012	0.068	-0.011	0.004	0.075

Table S3. Literature-supported comparison of cimetidine adsorption on nanocarriers

System	Adsorption Energy (eV)	Dominant Interaction	Structural Stability	Literature Basis
doped g-C_3N_4	−3.02 to −3.76	H-bonding +	High	Present

(this work)		electrostatic + charge transfer		study
Graphene oxide (GO)	~−0.5 to −2.5	H-bonding + vdW	Moderate	[41]
Carbon nanotubes (CNTs)	~−0.1 to −1.5	π–π stacking (physisorption)	High mechanical, low functional tunability	[42]
MOFs	~−0.5 to −4.5 (system dependent)	Coordination + electrostatic	Variable (often moisture sensitive)	literature consensus

Table S4. QTAIM topological parameters for Cmt adsorption on pristine and X-doped C_3N_4, including electron density ρ(r),

System	CP	Bond label	ρ (r)	$\nabla^2\rho$ (r)	G (r)	K (r)	V (r)	H (r)	G (r)/V(r)	ELF	Ɛ	λ_2	λ_3	λ_1/λ_3
Cmt-C_3N_4	147	C_{18}-O_{82}	0.67	0.26	0.55	-0.12	-0.43	0.12	-1.28	0.16	2.76	-0.13	0.33	-1.45
	137	C_{16}-N_{76}	0.54	0.21	0.40	-0.13	-0.27	0.13	-1.48	0.14	0.31	-0.16	0.25	-0.80
	107	N_{19}-O_{75}	0.11	0.44	0.45	-0.16	-0.79	0.16	-0.57	0.29	1.26	-0.39	0.57	-1.56
	181	C_{15}-H_{79}	0.18	0.79	0.14	-0.60	-0.77	0.60	-0.18	0.33	0.39	-0.46	0.90	-0.70
	198	N_{50}-H_{86}	0.50	0.11	0.33	0.54	-0.38	-0.54	-0.87	0.26	0.04	-0.85	0.28	-3.18
	100	N_{52}-N_{73}	0.28	0.95	0.20	-0.40	-0.16	0.40	-1.25	0.66	0.71	-0.95	0.12	-1.33
	117	N_{37}-H_{68}	0.14	0.39	0.89	-0.71	-0.82	0.71	-1.09	0.64	0.03	-0.14	0.67	-0.22
	156	N_{23}-C_{66}	0.57	0.19	0.37	-0.98	-0.27	0.98	-1.37	0.19	0.50	-0.23	0.25	-1.40
Cmt-P@C_3N_4	125	N_{36}-O_{75}	0.94	0.31	0.71	-0.80	-0.63	0.80	-1.13	0.28	0.07	-0.72	0.46	-1.67
	103	N_{52}-N_{73}	0.82	0.25	0.54	-0.79	-0.46	0.79	-1.17	0.31	0.57	-0.39	0.35	-1.74
	176	P_{54}-H_{86}	0.67	0.16	0.35	-0.37	-0.32	0.37	-1.09	0.35	0.13	-0.50	0.26	-2.15
Cmt-S@C_3N_4	211	N_{48}-H_{69}	0.31	0.11	0.22	-0.60	-0.16	0.60	-1.38	0.69	0.44	-0.18	0.16	-1.56
	199	N_{49}-C_{64}	0.65	0.21	0.41	-0.11	-0.29	0.11	-1.41	0.24	1.97	-0.15	0.27	-1.59

Laplacian $\nabla^2\rho$(r), kinetic energy density G(r), potential energy density V(r), and ellipticity ε at bond critical points. *All parameters are recorded in atomic units (a.u).*

	181	H_{22}-C_{65}	0.67	0.20	0.41	-0.96	-0.32	0.96	-1.28	0.26	1.93	-0.21	0.29	-2.10
	90	H_{27}-O_{75}	0.26	0.92	0.21	-0.25	-0.18	0.25	-1.17	0.97	0.03	-0.35	0.16	-2.31
	157	N_{44}-N_{67}	0.11	0.35	0.76	-0.10	-0.66	0.10	-1.15	0.45	0.11	-0.10	0.56	-0.20
Cmt-Si@C_3N_4	191	N_{49}-C_{64}	0.61	0.19	0.33	-0.97	-0.29	0.97	-1.14	0.23	0.13	-0.25	0.25	-1.57
	158	N_{53}-C_{63}	0.57	0.17	0.5	-0.67	-0.28	0.6	-1.79	0.21	1.41	-0.14	0.21	-1.50
	189	N_{50}-C_{65}	0.67	0.20	0.41	-0.83	-0.33	0.83	-1.24	0.27	0.59	-0.25	0.26	-1.47
	203	N_{43}-H_{71}	0.52	0.16	0.32	-0.77	-0.24	0.77	-1.33	0.20	2.57	-0.78	0.19	-1.37
	105	N_{47}-C_{172}	0.48	0.16	0.33	-0.60	-0.27	0.60	-1.22	0.14	1.20	-0.12	0.19	-2.03
	217	Si_{54}-H_{86}	0.86	0.19	0.43	-0.53	-0.38	0.53	-1.13	0.55	0.15	-0.56	0.32	-0.16
	205	N_{19}-O_{75}	0.11	0.46	0.98	-0.18	-0.80	0.18	-1.23	0.27	0.94	-0.54	0.61	-1.57
Cmt-B@C_3N_4	201	N_{49}-H_{70}	0.51	0.15	0.34	-0.46	-0.29	0.46	-1.17	0.16	0.18	-0.37	0.23	-1.91
	179	N_{21}-H_{71}	0.55	0.21	0.42	-0.11	-0.31	0.11	-1.35	0.14	0.36	-0.30	0.28	-1.46
	161	N_{44}-H_{67}	0.67	0.20	0.44	-0.73	-0.37	0.73	-1.19	0.24	0.03	-0.56	0.32	-1.81
	134	N_{45}-H_{86}	0.59	0.11	0.39	0.11	-0.50	-0.11	-0.78	0.31	0.03	-0.11	0.33	-0.33
	91	H_{27}-O_{75}	0.30	0.112	0.24	-0.27	-0.211	0.227	-1.14	0.11	0.03	--0.42	0.19	-2.32

Table S5. Molecular dynamics energy statistics for cimetidine (Cmt) adsorbed on pristine and X-doped C_3N_4 (X = B, P, S, Si) at simulation times of 100 ps, including total, potential, and kinetic energies, temperature, and their corresponding averages and standard deviations under NVT conditions at 298 K.

Cmt-C_3N_4					**Cmt-B@C_3N_4**				
Parameters	Initial energy	Final energy	Average	Standard deviation	Parameters	Initial energy	Final energy	Average	Standard deviation
Tot. energy (kcal/mol)	11898.32	15232.67	15400.73	11898.32	Tot. energy (kcal/mol)	12906.68	15287.7	15554	598.648
Pot. energy (kcal/mol)	6658.353	9911.045	10160.83	6658.353	Pot. energy (kcal/mol)	7666.719	10151.71	10314.01	414.577
Kin. energy (kcal/mol)	5239.965	5321.624	5239.892	5239.965	Kin. energy (kcal/mol)	5239.965	5135.99	5239.999	261.04
Temperature (K)	298	302.644	297.996	15.445	Temperature (K)	298	292.087	298.002	14.845
Cmt-P@C_3N_4					**Cmt-S@C_3N_4**				
Parameters	Initial energy	Final energy	Average	Standard deviation	Parameters	Initial energy	Final energy	Average	Standard deviation
Tot. energy (kcal/mol)	65366.64	15544.07	15729.78	1306.262	Tot. energy (kcal/mol)	14059.57	17412.11	17499.65	594.64
Pot. energy (kcal/mol)	60126.68	10262.95	10489.82	879.032	Pot. energy (kcal/mol)	8819.606	12024.91	12259.72	395.498
Kin. energy (kcal/mol)	5239.965	5281.121	5239.965	569.108	Kin. energy (kcal/mol)	5239.965	5387.205	5239.926	266.82
Temperature (K)	298	300.341	298	32.366	Temperature (K)	298	306.374	297.998	15.174
Cmt-Si@C_3N_4									
Parameters	Initial energy	Final energy	Average	Standard deviation					
Tot. energy (kcal/mol)	11299.34	14830.03	15046.53	588.015					
Pot. energy (kcal/mol)	6059.375	9575.306	9806.558	371.34					
Kin. energy (kcal/mol)	5239.965	5254.723	5239.976	272.66					
Temperature (K)	298	298.839	298.001	15.506					

Table S6. Molecular dynamics energy parameters for cimetidine (Cmt) adsorbed on pristine and X-doped C_3N_4 surfaces (X = B, P, S, Si) obtained from 500 ps NVT simulations at 298 K, showing initial, final, and average values of total, potential, and kinetic energies, as well as temperature and corresponding standard deviations, calculated using the Universal Force Field (UFF).

Cmt-C_3N_4					**Cmt-B@C_3N_4**				
Parameters	Initial energy	Final energy	Average	Standard deviation	Parameters	Initial energy	Final energy	Average	Standard deviation
Tot. energy (kcal/mol)	11898.32	15016.01	15121.2	605.835	Tot. energy (kcal/mol)	12906.68	15125.58	15301.54	354.006
Pot. energy (kcal/mol)	6658.353	9765.863	9881.237	403.077	Pot. energy (kcal/mol)	7666.719	9867.696	10061.58	291.304
Kin. energy (kcal/mol)	5239.965	5250.144	5239.96	271.579	Kin. energy (kcal/mol)	5239.965	5257.883	5239.962	127.82
Temperature (K)	298	298.579	298	7.498	Temperature (K)	298	299.019	298	7.269
Cmt-P@C_3N_4					**Cmt-S@C_3N_4**				
Parameters	Initial energy	Final energy	Average	Standard deviation	Parameters	Initial energy	Final energy	Average	Standard deviation
Tot. energy (kcal/mol)	65366.64	15163.13	15331.26	601.117	Tot. energy (kcal/mol)	14059.57	17051.38	17181.6	331.84
Pot. energy (kcal/mol)	60126.68	9939.985	10091.3	414.439	Pot. energy (kcal/mol)	8819.606	11782.82	11941.63	254.832
Kin. energy (kcal/mol)	5239.965	5223.14	5239.958	261.208	Kin. energy (kcal/mol)	5239.965	5268.561	5239.967	133.759
Temperature (K)	298	297.043	298	14.855	Temperature (K)	298	299.626	298	7.607
Cmt-Si@C_3N_4									
Parameters	Initial energy	Final energy	Average	Standard deviation					
Tot. energy (kcal/mol)	11299.34	14493.4	14688.06	340.046					
Pot. energy (kcal/mol)	6059.375	9291.734	9448.091	269.642					
Kin. energy (kcal/mol)	5239.965	5201.665	5239.965	130.772					
Temperature (K)	298	295.822	298	7.437					